



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 01:35 pm BST

PDB ID : 8RTR / pdb_00008rtr
Title : Bilirubin oxidase from Myrothecium verrucaria with R356S mutation
Authors : Svecova, L.; Koval, T.; Kolenko, P.; Ostergaard, L.H.; Dohnalek, J.
Deposited on : 2024-01-27
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

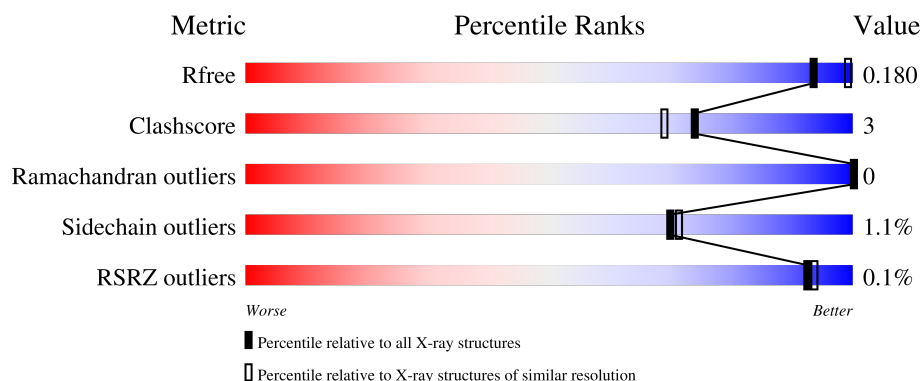
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



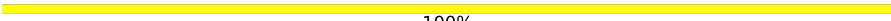
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	534	 90% 9% .
1	BBB	534	 92% 7%
2	AeA	3	 67% 33%
2	BeB	3	 100%
3	AhA	2	 100%

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Mol	Chain	Length	Quality of chain
3	BhB	2	 100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9994 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

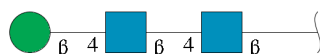
- Molecule 1 is a protein called Bilirubin oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	534	Total	C	N	O	S	0	12	0
			4305	2752	728	811	14			
1	BBB	533	Total	C	N	O	S	0	8	0
			4272	2730	722	806	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	356	SER	ARG	engineered mutation	UNP Q12737
BBB	356	SER	ARG	engineered mutation	UNP Q12737

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AeA	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	BeB	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

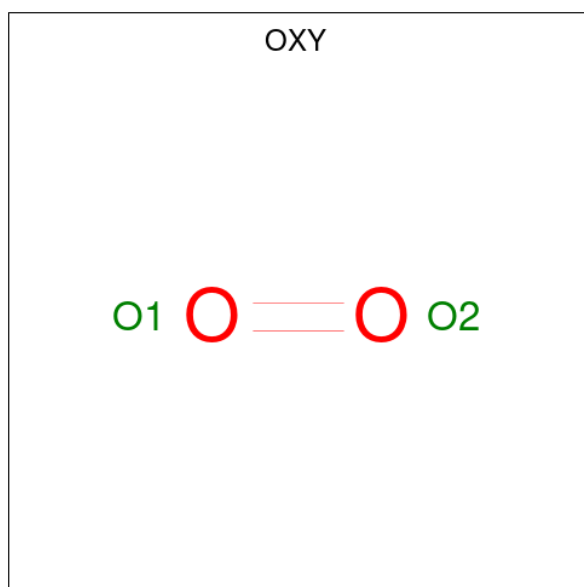


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AhA	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	BhB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	4	Total	Cu	0	0
			4	4		
4	BBB	4	Total	Cu	0	0
			4	4		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	O	0	0
			2	2		
5	BBB	1	Total	O	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



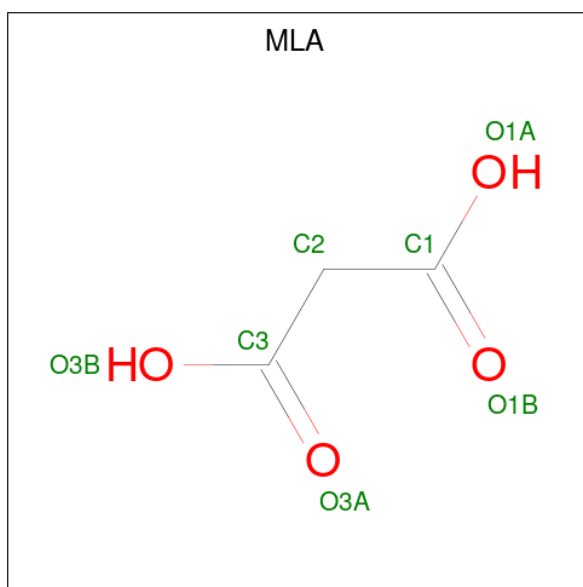
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			6	3	3		
6	AAA	1	Total	C	O	0	0
			6	3	3		
6	AAA	1	Total	C	O	0	0
			6	3	3		
6	AAA	1	Total	C	O	0	0
			6	3	3		
6	BBB	1	Total	C	O	0	0
			6	3	3		
6	BBB	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			10	6	4		
7	AAA	1	Total	C	O	0	0
			10	6	4		
7	BBB	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total	C	O	0	0
			7	3	4		
8	AAA	1	Total	C	O	0	0
			7	3	4		
8	BBB	1	Total	C	O	0	0
			7	3	4		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	5	Total	Cl	0	0
			5	5		
9	BBB	4	Total	Cl	0	0
			4	4		

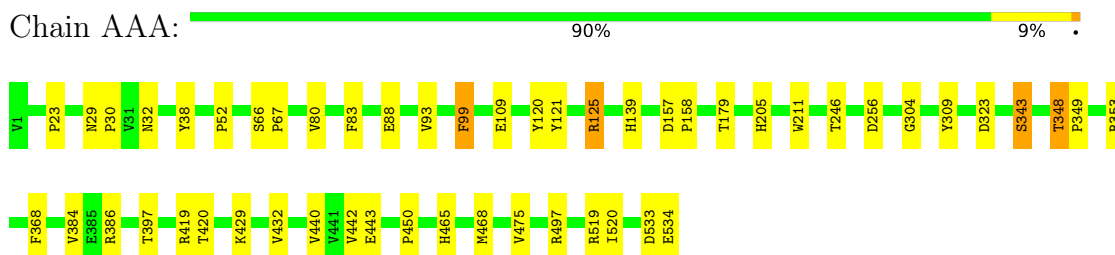
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	595	Total	O	0	6
			596	596		
10	BBB	565	Total	O	0	2
			566	566		

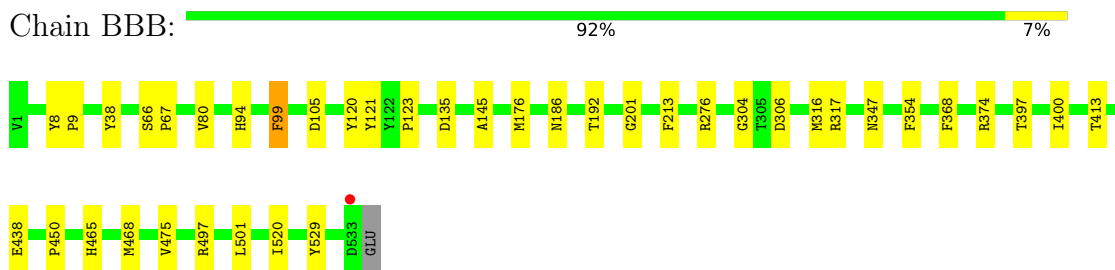
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

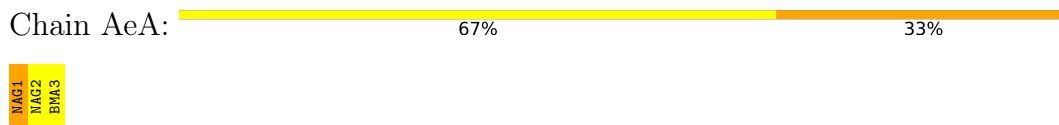
- Molecule 1: Bilirubin oxidase



- Molecule 1: Bilirubin oxidase



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AhA:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BhB:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.07Å 200.89Å 217.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.05 47.78 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.78-2.05) 98.9 (47.78-2.05)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.158 , 0.203 0.169 , 0.180	Depositor DCC
R_{free} test set	4479 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9994	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CU, MLA, OXY, CL, NAG, BMA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AAA	1.05	3/4472 (0.1%)	1.24	6/6112 (0.1%)
1	BBB	1.05	0/4428	1.26	8/6056 (0.1%)
All	All	1.05	3/8900 (0.0%)	1.25	14/12168 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	139	HIS	CE1-NE2	5.53	1.38	1.32
1	AAA	30	PRO	C-O	-5.28	1.17	1.24
1	AAA	23	PRO	C-O	-5.23	1.17	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	99	PHE	CA-CB-CG	7.86	121.66	113.80
1	AAA	99	PHE	CA-CB-CG	6.59	120.39	113.80
1	AAA	246	THR	CA-CB-OG1	-6.05	100.52	109.60
1	AAA	348	THR	CB-CA-C	5.83	119.25	109.69
1	AAA	533	ASP	CA-CB-CG	5.71	118.31	112.60
1	BBB	192	THR	N-CA-C	-5.42	106.67	113.28
1	BBB	145	ALA	CA-C-N	5.28	127.36	120.28
1	BBB	145	ALA	C-N-CA	5.28	127.36	120.28
1	BBB	501	LEU	CA-C-N	5.17	125.72	119.98
1	BBB	501	LEU	C-N-CA	5.17	125.72	119.98
1	AAA	349	PRO	CB-CA-C	-5.07	104.74	111.23
1	AAA	211	TRP	O-C-N	-5.05	119.21	121.53
1	BBB	135	ASP	CA-CB-CG	-5.03	107.57	112.60
1	BBB	347	ASN	CA-CB-CG	-5.01	107.59	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4305	0	4116	31	0
1	BBB	4272	0	4065	17	0
2	AeA	39	0	34	1	0
2	BeB	39	0	34	0	0
3	AhA	28	0	25	0	0
3	BhB	28	0	25	0	0
4	AAA	4	0	0	0	0
4	BBB	4	0	0	0	0
5	AAA	2	0	0	0	0
5	BBB	2	0	0	0	0
6	AAA	30	0	40	3	0
6	BBB	12	0	16	1	0
7	AAA	20	0	28	5	0
7	BBB	10	0	14	0	0
8	AAA	21	0	6	3	0
8	BBB	7	0	2	0	0
9	AAA	5	0	0	0	0
9	BBB	4	0	0	0	0
10	AAA	596	0	0	10	0
10	BBB	566	0	0	3	0
All	All	9994	0	8405	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:125[A]:ARG:HH11	1:AAA:125[A]:ARG:HG3	1.48	0.77
1:AAA:88[B]:GLU:OE2	1:AAA:88[B]:GLU:HA	1.85	0.76
1:BBB:497:ARG:HD3	10:BBB:711:HOH:O	1.90	0.69
1:AAA:465:HIS:ND1	10:AAA:701:HOH:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:534:GLU:OE2	1:AAA:534:GLU:HA	2.00	0.62
7:AAA:612:PGE:H1	10:AAA:1139:HOH:O	2.00	0.61
1:AAA:353[A]:ARG:HD3	10:AAA:792[A]:HOH:O	2.00	0.60
1:AAA:304:GLY:HA2	1:AAA:397:THR:HG21	1.83	0.59
1:AAA:157:ASP:OD2	8:AAA:615:MLA:O1B	2.22	0.57
1:AAA:323:ASP:HB3	10:AAA:1025:HOH:O	2.07	0.55
1:BBB:201:GLY:H	6:BBB:606:GOL:H31	1.74	0.52
1:AAA:432:VAL:HG21	1:AAA:440:VAL:HG11	1.92	0.51
1:AAA:158:PRO:HD2	10:AAA:1090:HOH:O	2.11	0.51
1:AAA:419:ARG:HA	7:AAA:612:PGE:H4	1.92	0.51
1:BBB:186:ASN:HB3	10:BBB:1102:HOH:O	2.11	0.50
1:BBB:304:GLY:HA2	1:BBB:397:THR:HG21	1.92	0.50
1:BBB:66:SER:HA	1:BBB:67:PRO:C	2.37	0.48
1:AAA:109:GLU:HG3	10:AAA:1094:HOH:O	2.13	0.48
1:BBB:465:HIS:ND1	10:BBB:705:HOH:O	2.36	0.47
7:AAA:612:PGE:C1	10:AAA:1139:HOH:O	2.61	0.47
1:AAA:497:ARG:HH22	1:AAA:519[B]:ARG:HH11	1.62	0.46
1:AAA:38:TYR:CD1	1:AAA:520:ILE:HD11	2.50	0.46
6:AAA:610:GOL:H12	10:AAA:970:HOH:O	2.16	0.46
1:AAA:443:GLU:OE2	8:AAA:613:MLA:O3B	2.34	0.46
1:AAA:343:SER:O	1:AAA:384:VAL:HG11	2.16	0.46
1:AAA:386:ARG:HD2	10:AAA:827:HOH:O	2.15	0.45
1:AAA:80:VAL:HA	1:AAA:120:TYR:O	2.16	0.45
1:AAA:420:THR:H	7:AAA:612:PGE:H32	1.80	0.45
1:BBB:8:TYR:CD2	1:BBB:9:PRO:HD2	2.52	0.45
1:BBB:80:VAL:HA	1:BBB:120:TYR:O	2.18	0.44
1:BBB:450:PRO:HB3	1:BBB:475:VAL:HG13	2.00	0.43
1:AAA:125[A]:ARG:HH22	8:AAA:614:MLA:HC21	1.83	0.43
1:AAA:256:ASP:HB2	1:AAA:429:LYS:HA	2.00	0.43
1:AAA:386:ARG:HA	1:AAA:442:VAL:O	2.18	0.43
1:AAA:450:PRO:HB3	1:AAA:475:VAL:HG13	2.01	0.42
1:BBB:413:THR:O	1:BBB:438:GLU:HA	2.19	0.42
1:BBB:38:TYR:CD1	1:BBB:520:ILE:HD11	2.54	0.42
1:BBB:354:PHE:CE2	1:BBB:400:ILE:HD12	2.54	0.42
1:BBB:123:PRO:HB3	1:BBB:529:TYR:CG	2.53	0.42
1:AAA:419:ARG:HB2	7:AAA:612:PGE:H4	2.01	0.42
6:AAA:610:GOL:H31	2:AeA:1:NAG:C8	2.49	0.42
1:BBB:368:PHE:HB2	1:BBB:468:MET:HB3	2.02	0.42
1:AAA:29:ASN:HB3	1:AAA:32:ASN:OD1	2.20	0.42
1:AAA:52:PRO:HA	10:AAA:1131:HOH:O	2.19	0.42
1:AAA:179:THR:OG1	1:AAA:205:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:66:SER:HA	1:AAA:67:PRO:C	2.44	0.41
1:AAA:368:PHE:HB2	1:AAA:468:MET:HB3	2.01	0.41
1:BBB:213:PHE:HA	1:BBB:317:ARG:O	2.20	0.41
1:AAA:83:PHE:CG	1:AAA:93:VAL:HG21	2.56	0.41
1:AAA:309:TYR:OH	6:AAA:606:GOL:H31	2.20	0.41
1:BBB:94:HIS:ND1	1:BBB:105:ASP:O	2.52	0.40
1:BBB:176:MET:HE1	1:BBB:316:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	544/534 (102%)	518 (95%)	26 (5%)	0	100	100
1	BBB	539/534 (101%)	506 (94%)	33 (6%)	0	100	100
All	All	1083/1068 (101%)	1024 (95%)	59 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	465/453 (103%)	459 (99%)	6 (1%)	65	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BBB	460/453 (102%)	455 (99%)	5 (1%)	70	71
All	All	925/906 (102%)	914 (99%)	11 (1%)	70	68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	99	PHE
1	AAA	121	TYR
1	AAA	125[A]	ARG
1	AAA	125[B]	ARG
1	AAA	343	SER
1	AAA	348	THR
1	BBB	99	PHE
1	BBB	121	TYR
1	BBB	276	ARG
1	BBB	306	ASP
1	BBB	374	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	AeA	1	2,1	14,14,15	1.24	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	AeA	2	2	14,14,15	0.62	0	17,19,21	1.58	4 (23%)
2	BMA	AeA	3	2	11,11,12	0.75	0	15,15,17	2.40	5 (33%)
3	NAG	AhA	1	1,3	14,14,15	0.78	0	17,19,21	0.95	1 (5%)
3	NAG	AhA	2	3	14,14,15	1.00	0	17,19,21	2.25	7 (41%)
2	NAG	BeB	1	2,1	14,14,15	0.74	0	17,19,21	1.32	2 (11%)
2	NAG	BeB	2	2	14,14,15	0.67	0	17,19,21	1.35	4 (23%)
2	BMA	BeB	3	2	11,11,12	1.03	0	15,15,17	2.32	6 (40%)
3	NAG	BhB	1	1,3	14,14,15	0.65	0	17,19,21	1.23	2 (11%)
3	NAG	BhB	2	3	14,14,15	0.96	1 (7%)	17,19,21	1.64	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	AeA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AeA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AeA	3	2	-	2/2/19/22	0/1/1/1
3	NAG	AhA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	AhA	2	3	-	2/6/23/26	0/1/1/1
2	NAG	BeB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	BeB	2	2	-	0/6/23/26	0/1/1/1
2	BMA	BeB	3	2	-	2/2/19/22	0/1/1/1
3	NAG	BhB	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	BhB	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AeA	1	NAG	C2-N2	-3.24	1.40	1.46
3	BhB	2	NAG	C1-C2	2.72	1.56	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AeA	3	BMA	O5-C5-C6	5.49	115.81	107.20
2	BeB	3	BMA	O5-C5-C6	5.33	115.56	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AhA	2	NAG	C1-O5-C5	5.06	119.05	112.19
3	AhA	2	NAG	O4-C4-C5	4.28	119.93	109.30
2	BeB	3	BMA	C3-C4-C5	3.99	117.36	110.24
2	AeA	3	BMA	C3-C4-C5	3.75	116.94	110.24
3	BhB	2	NAG	C1-O5-C5	3.62	117.09	112.19
2	AeA	3	BMA	C1-C2-C3	3.34	113.78	109.67
3	AhA	2	NAG	O5-C5-C6	-3.08	102.38	107.20
2	BeB	3	BMA	C1-O5-C5	3.04	116.31	112.19
2	BeB	1	NAG	O4-C4-C3	-3.00	103.41	110.35
2	BeB	2	NAG	C3-C4-C5	-2.99	104.90	110.24
2	BeB	1	NAG	O5-C5-C6	-2.88	102.69	107.20
3	BhB	2	NAG	O4-C4-C5	2.87	116.43	109.30
2	AeA	2	NAG	C8-C7-N2	-2.84	111.29	116.10
3	AhA	2	NAG	O5-C1-C2	-2.80	106.87	111.29
2	AeA	2	NAG	C1-O5-C5	2.78	115.96	112.19
2	AeA	3	BMA	C1-O5-C5	2.75	115.92	112.19
2	BeB	3	BMA	O6-C6-C5	2.73	120.67	111.29
3	BhB	2	NAG	C1-C2-N2	2.64	114.99	110.49
3	AhA	2	NAG	C3-C4-C5	-2.63	105.56	110.24
3	BhB	1	NAG	O5-C5-C6	2.47	111.07	107.20
2	AeA	2	NAG	O4-C4-C5	2.37	115.17	109.30
2	AeA	3	BMA	O6-C6-C5	2.34	119.32	111.29
2	BeB	3	BMA	C6-C5-C4	-2.34	107.53	113.00
2	BeB	3	BMA	O4-C4-C3	-2.29	105.06	110.35
3	AhA	2	NAG	C8-C7-N2	-2.28	112.25	116.10
2	AeA	2	NAG	O5-C1-C2	-2.27	107.70	111.29
2	AeA	1	NAG	O4-C4-C3	-2.23	105.19	110.35
3	AhA	2	NAG	C1-C2-N2	2.15	114.16	110.49
3	BhB	1	NAG	C8-C7-N2	-2.10	112.55	116.10
2	BeB	2	NAG	O4-C4-C5	2.09	114.49	109.30
2	BeB	2	NAG	C2-N2-C7	2.07	125.86	122.90
3	AhA	1	NAG	C4-C3-C2	2.07	114.05	111.02
2	BeB	2	NAG	C1-O5-C5	2.03	114.94	112.19
3	BhB	2	NAG	C3-C4-C5	-2.02	106.64	110.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BeB	3	BMA	O5-C5-C6-O6
2	AeA	3	BMA	O5-C5-C6-O6
2	BeB	3	BMA	C4-C5-C6-O6

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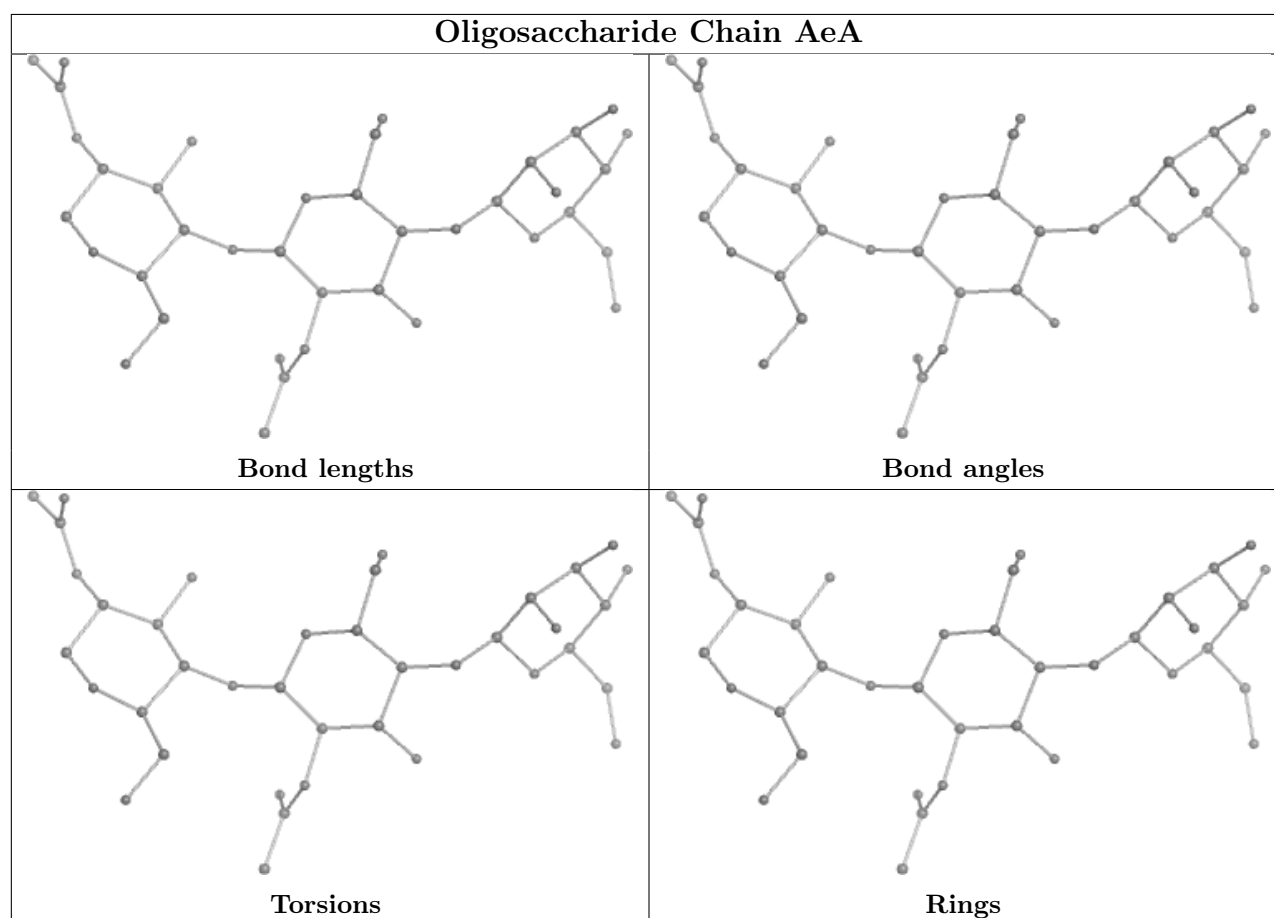
Mol	Chain	Res	Type	Atoms
2	AeA	3	BMA	C4-C5-C6-O6
3	AhA	2	NAG	O5-C5-C6-O6
3	AhA	2	NAG	C4-C5-C6-O6
3	BhB	2	NAG	C4-C5-C6-O6
3	BhB	2	NAG	O5-C5-C6-O6

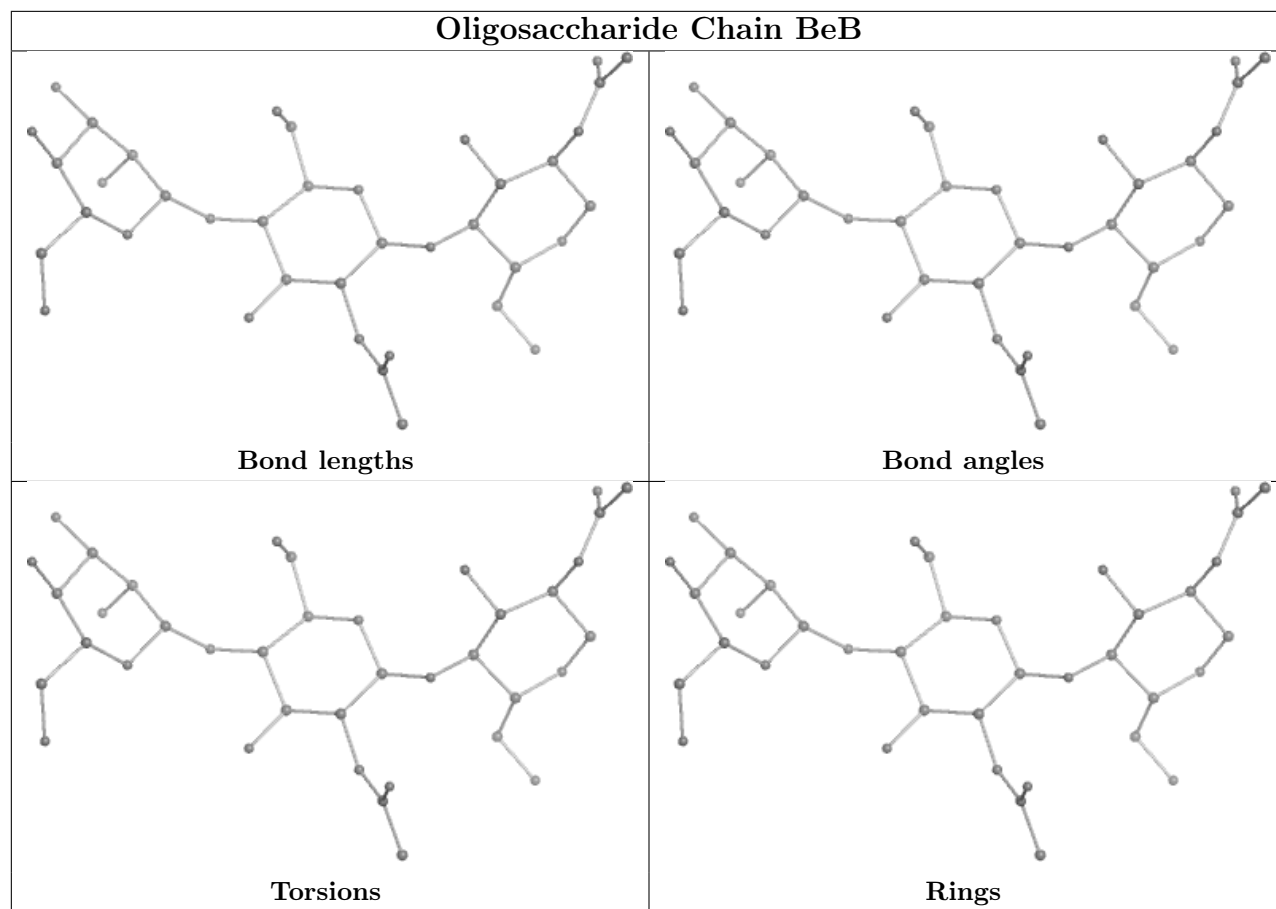
There are no ring outliers.

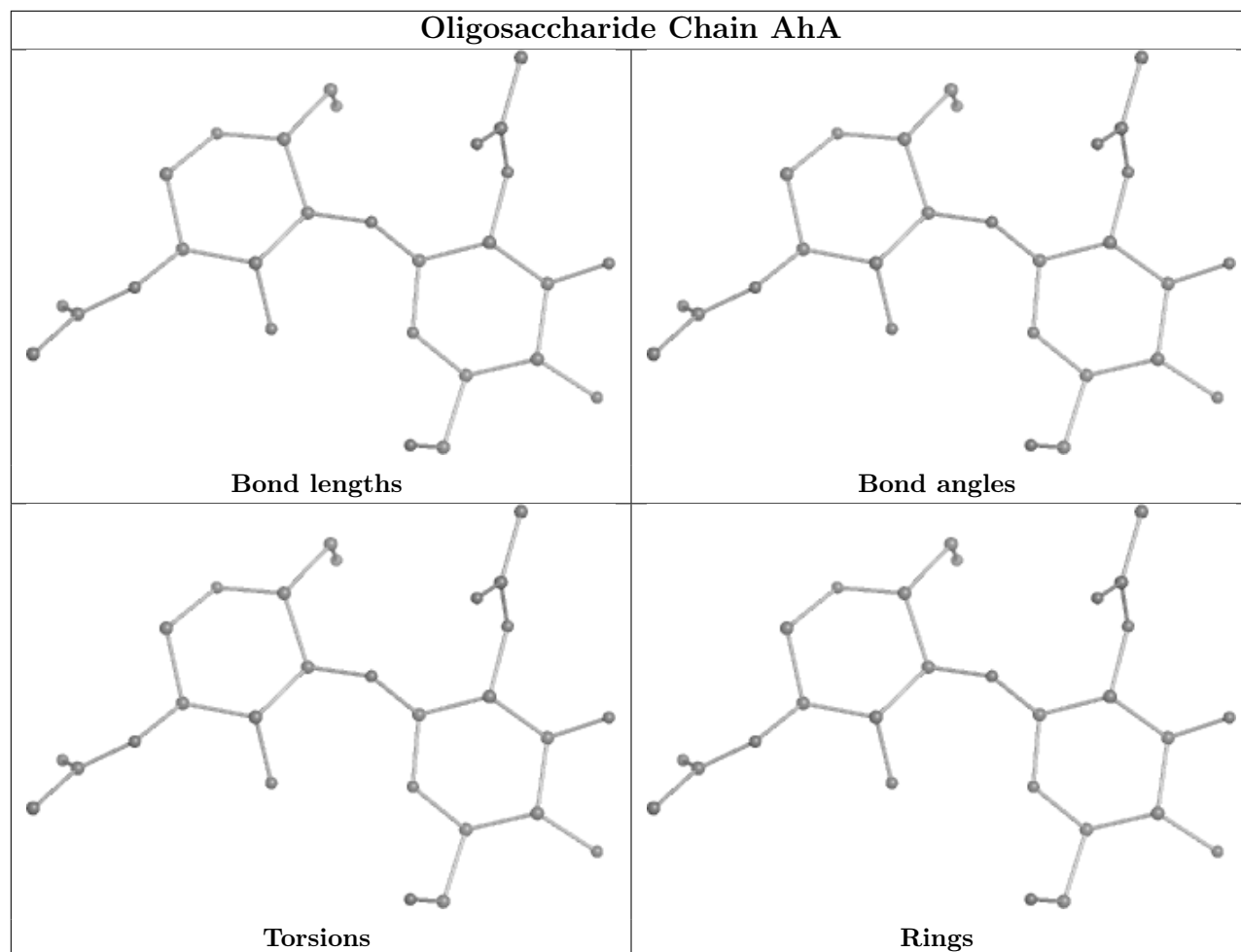
1 monomer is involved in 1 short contact:

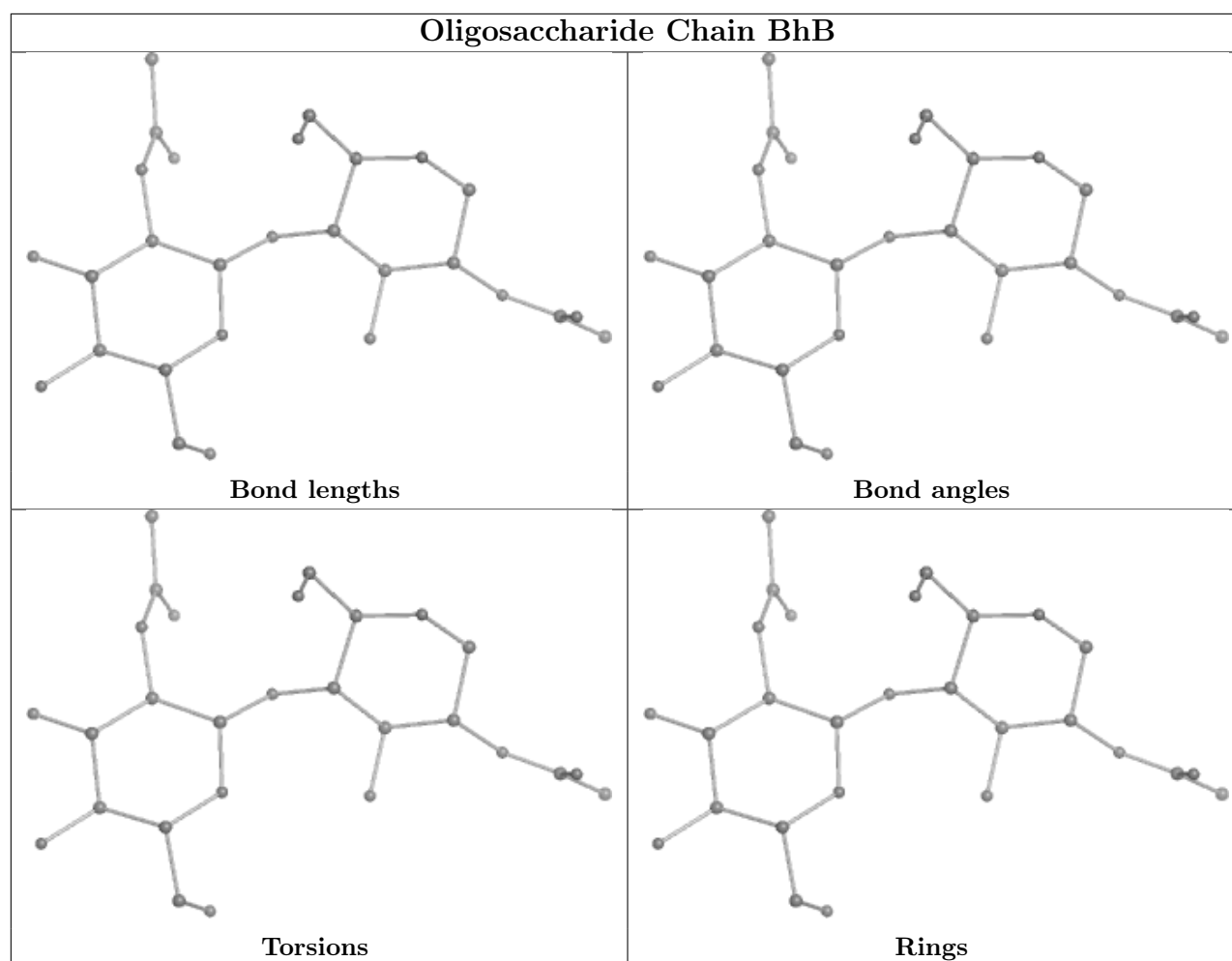
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AeA	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 17 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PGE	AAA	611	-	9,9,9	0.20	0	8,8,8	0.25	0
6	GOL	AAA	606	-	5,5,5	0.26	0	5,5,5	0.65	0
5	OXY	AAA	605	4	1,1,1	0.63	0	-		
5	OXY	BBB	605	4	1,1,1	0.50	0	-		
6	GOL	BBB	606	-	5,5,5	0.18	0	5,5,5	0.35	0
7	PGE	BBB	608	-	9,9,9	0.25	0	8,8,8	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	AAA	608	-	5,5,5	0.15	0	5,5,5	0.46	0
6	GOL	AAA	610	-	5,5,5	0.31	0	5,5,5	0.72	0
8	MLA	AAA	613	-	6,6,6	1.40	0	7,7,7	0.92	0
8	MLA	AAA	615	-	6,6,6	1.63	2 (33%)	7,7,7	1.17	0
6	GOL	AAA	607	-	5,5,5	0.26	0	5,5,5	0.50	0
8	MLA	AAA	614	-	6,6,6	2.10	4 (66%)	7,7,7	1.09	0
6	GOL	BBB	607	-	5,5,5	0.15	0	5,5,5	0.42	0
8	MLA	BBB	609	-	6,6,6	1.24	1 (16%)	7,7,7	1.12	0
6	GOL	AAA	609	-	5,5,5	0.14	0	5,5,5	0.42	0
7	PGE	AAA	612	-	9,9,9	0.34	0	8,8,8	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	AAA	611	-	-	1/7/7/7	-
6	GOL	AAA	606	-	-	2/4/4/4	-
7	PGE	BBB	608	-	-	3/7/7/7	-
6	GOL	BBB	606	-	-	2/4/4/4	-
8	MLA	AAA	615	-	-	1/4/4/4	-
8	MLA	AAA	613	-	-	2/4/4/4	-
6	GOL	AAA	608	-	-	4/4/4/4	-
6	GOL	AAA	610	-	-	2/4/4/4	-
6	GOL	AAA	607	-	-	3/4/4/4	-
8	MLA	AAA	614	-	-	0/4/4/4	-
6	GOL	BBB	607	-	-	2/4/4/4	-
8	MLA	BBB	609	-	-	2/4/4/4	-
6	GOL	AAA	609	-	-	4/4/4/4	-
7	PGE	AAA	612	-	-	3/7/7/7	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AAA	614	MLA	C2-C1	2.80	1.55	1.51
8	AAA	614	MLA	C2-C3	2.80	1.55	1.51
8	AAA	615	MLA	O1A-C1	-2.43	1.22	1.30
8	AAA	614	MLA	O3B-C3	-2.40	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AAA	615	MLA	O3B-C3	-2.30	1.23	1.30
8	AAA	614	MLA	O1A-C1	-2.12	1.23	1.30
8	BBB	609	MLA	O1A-C1	-2.05	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	608	GOL	O1-C1-C2-C3
6	AAA	608	GOL	C1-C2-C3-O3
6	AAA	610	GOL	C1-C2-C3-O3
6	AAA	610	GOL	O2-C2-C3-O3
6	BBB	606	GOL	C1-C2-C3-O3
6	BBB	606	GOL	O2-C2-C3-O3
6	BBB	607	GOL	O1-C1-C2-C3
6	AAA	608	GOL	O2-C2-C3-O3
7	AAA	612	PGE	O3-C5-C6-O4
6	AAA	606	GOL	O1-C1-C2-C3
6	AAA	607	GOL	C1-C2-C3-O3
6	AAA	609	GOL	O1-C1-C2-C3
6	AAA	609	GOL	C1-C2-C3-O3
6	AAA	606	GOL	O1-C1-C2-O2
6	AAA	607	GOL	O2-C2-C3-O3
6	AAA	609	GOL	O1-C1-C2-O2
6	BBB	607	GOL	O1-C1-C2-O2
7	BBB	608	PGE	C4-C3-O2-C2
8	AAA	613	MLA	O1A-C1-C2-C3
7	AAA	611	PGE	O1-C1-C2-O2
8	AAA	613	MLA	O1B-C1-C2-C3
7	AAA	612	PGE	C1-C2-O2-C3
7	BBB	608	PGE	O1-C1-C2-O2
7	AAA	612	PGE	C4-C3-O2-C2
6	AAA	609	GOL	O2-C2-C3-O3
8	BBB	609	MLA	C1-C2-C3-O3A
8	BBB	609	MLA	C1-C2-C3-O3B
6	AAA	608	GOL	O1-C1-C2-O2
6	AAA	607	GOL	O1-C1-C2-O2
7	BBB	608	PGE	C3-C4-O3-C5
8	AAA	615	MLA	C1-C2-C3-O3A

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	606	GOL	1	0
6	BBB	606	GOL	1	0
6	AAA	610	GOL	2	0
8	AAA	613	MLA	1	0
8	AAA	615	MLA	1	0
8	AAA	614	MLA	1	0
7	AAA	612	PGE	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	534/534 (100%)	-0.65	0 100 100	13, 23, 37, 74	12 (2%)
1	BBB	533/534 (99%)	-0.54	1 (0%) 92 93	17, 28, 41, 57	8 (1%)
All	All	1067/1068 (99%)	-0.60	1 (0%) 92 94	13, 26, 40, 74	20 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	533	ASP	2.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	AeA	1	14/15	-	-	26,29,35,39	0
2	NAG	AeA	2	14/15	-	-	35,47,62,72	0
2	BMA	AeA	3	11/12	-	-	81,88,93,95	0
2	NAG	BeB	1	14/15	-	-	29,33,40,42	0
2	NAG	BeB	2	14/15	-	-	47,56,68,79	0
2	BMA	BeB	3	11/12	-	-	86,90,104,106	0
3	NAG	AhA	1	14/15	-	-	24,28,31,34	0
3	NAG	AhA	2	14/15	-	-	36,46,55,55	0

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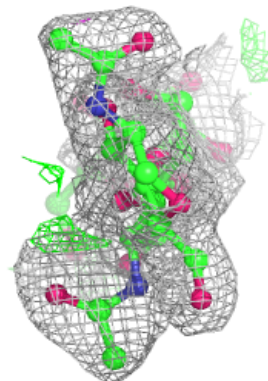
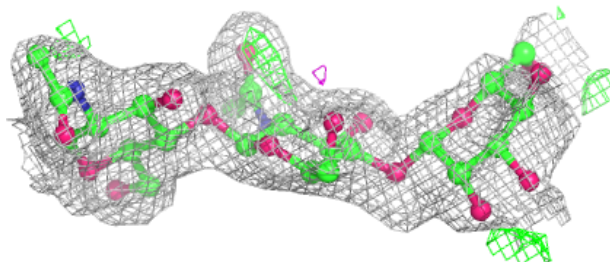
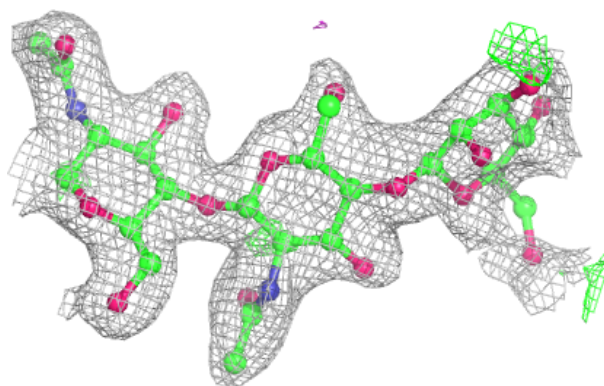
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	BhB	1	14/15	-	-	27,31,34,38	0
3	NAG	BhB	2	14/15	-	-	42,48,59,62	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

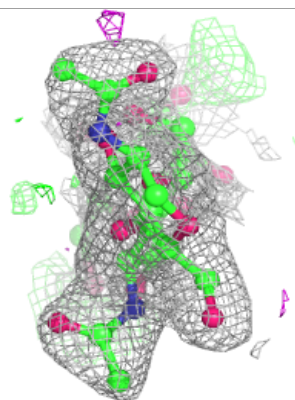
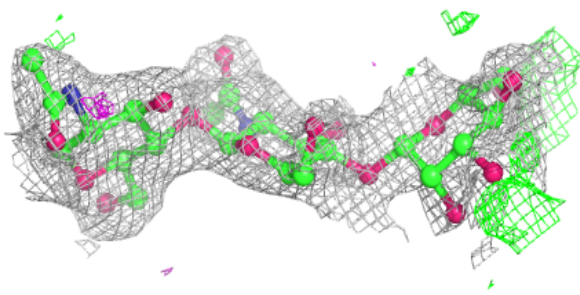
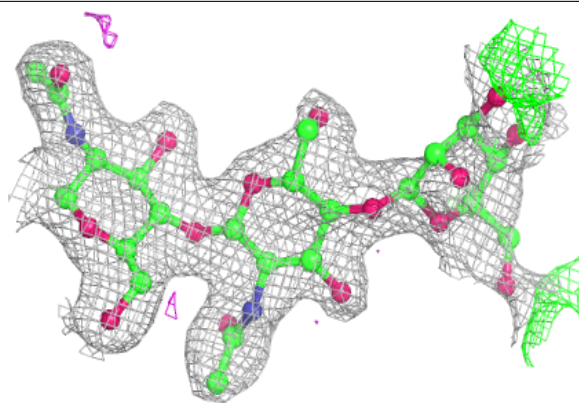
Electron density around Chain AeA:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



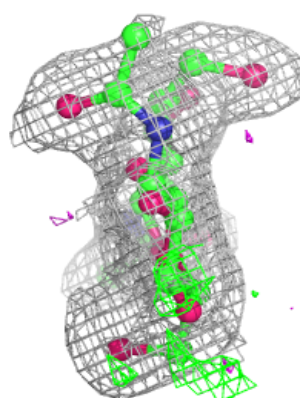
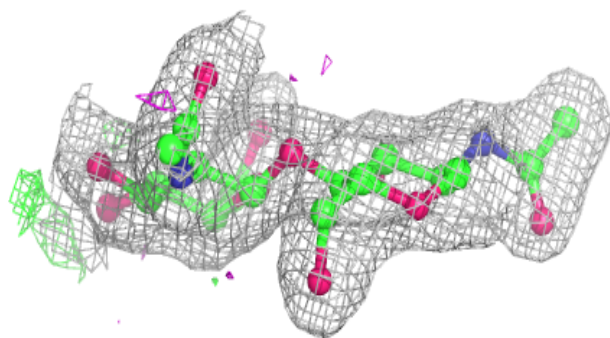
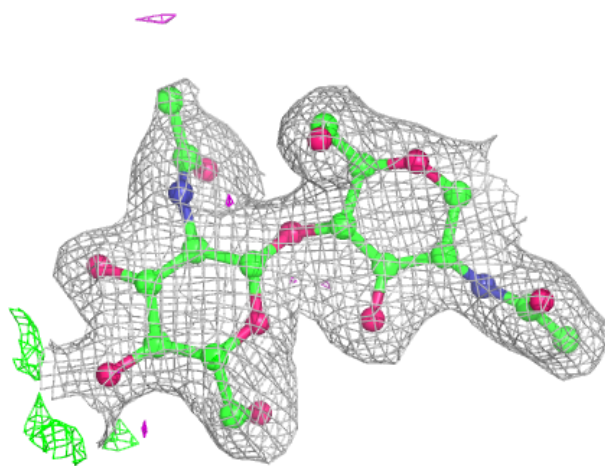
Electron density around Chain BeB:

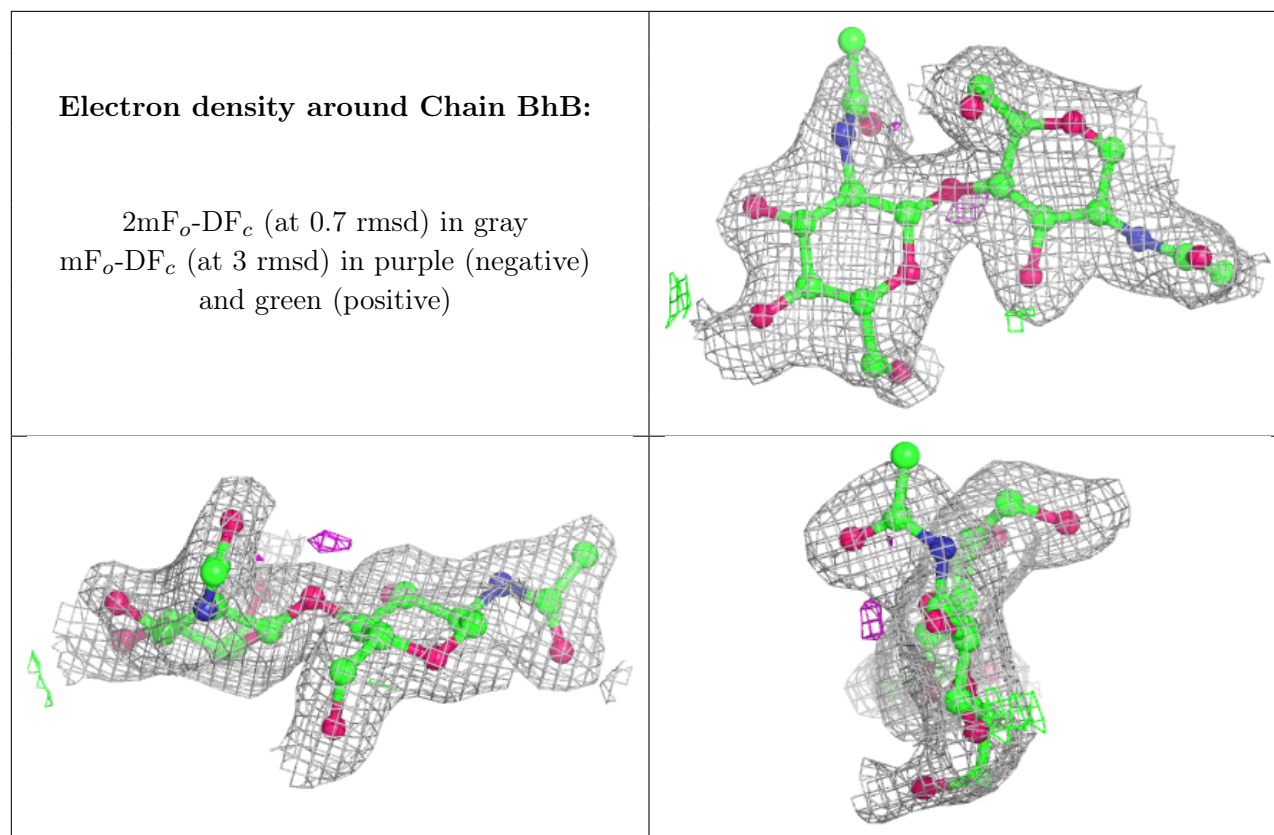
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain AhA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	AAA	607	6/6	0.83	0.15	43,45,54,54	0
7	PGE	AAA	612	10/10	0.86	0.17	54,59,63,64	0
6	GOL	AAA	609	6/6	0.90	0.11	44,55,58,60	0
6	GOL	AAA	606	6/6	0.91	0.11	37,41,46,47	0
6	GOL	AAA	610	6/6	0.92	0.12	36,41,44,50	0
8	MLA	AAA	613	7/7	0.92	0.09	40,49,60,75	0
8	MLA	BBB	609	7/7	0.92	0.10	32,38,53,71	0
6	GOL	AAA	608	6/6	0.93	0.10	43,51,54,57	0
8	MLA	AAA	614	7/7	0.93	0.11	29,49,53,58	0
7	PGE	BBB	608	10/10	0.93	0.11	47,51,54,57	0
6	GOL	BBB	606	6/6	0.94	0.10	34,43,45,47	0
7	PGE	AAA	611	10/10	0.95	0.09	42,47,51,59	0
6	GOL	BBB	607	6/6	0.95	0.09	45,53,53,53	0
8	MLA	AAA	615	7/7	0.96	0.07	33,39,45,47	0

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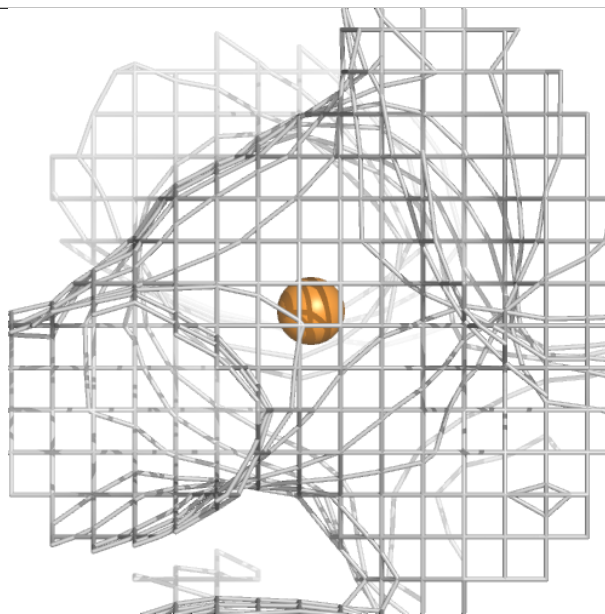
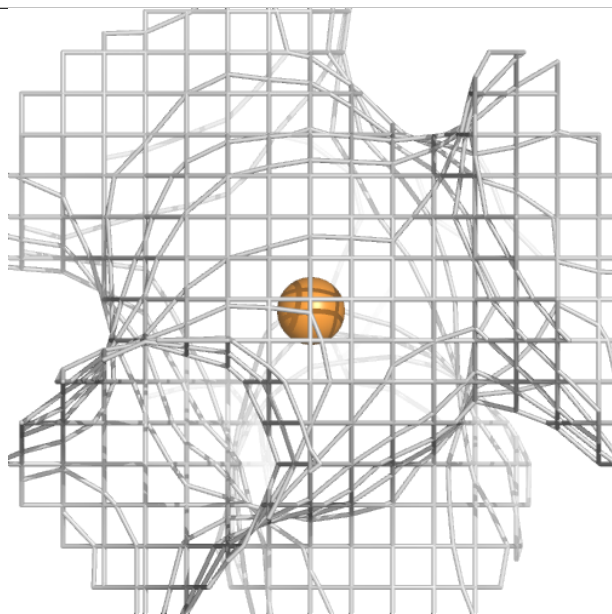
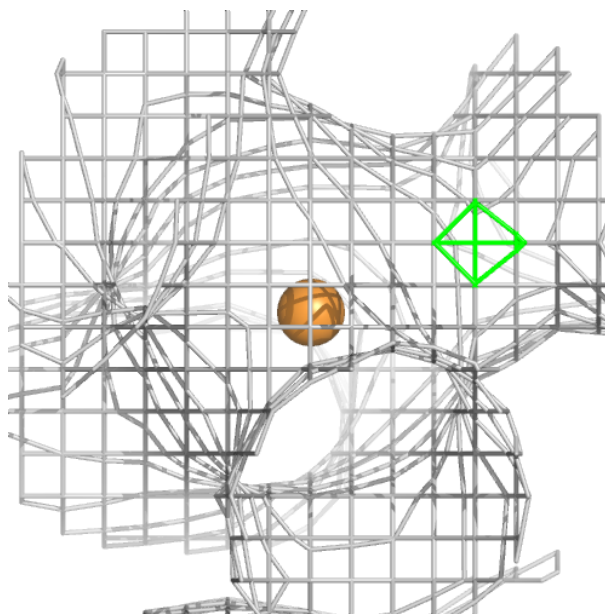
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CL	AAA	617	1/1	0.98	0.07	44,44,44,44	0
9	CL	BBB	610	1/1	0.98	0.07	36,36,36,36	0
9	CL	AAA	616	1/1	0.99	0.05	34,34,34,34	0
5	OXY	AAA	605	2/2	0.99	0.03	15,15,15,17	0
9	CL	AAA	618	1/1	0.99	0.08	27,27,27,27	0
9	CL	AAA	619	1/1	0.99	0.15	41,41,41,41	0
9	CL	AAA	620	1/1	0.99	0.14	46,46,46,46	0
5	OXY	BBB	605	2/2	0.99	0.03	20,20,20,21	0
9	CL	BBB	611	1/1	0.99	0.04	35,35,35,35	0
9	CL	BBB	612	1/1	0.99	0.06	50,50,50,50	0
9	CL	BBB	613	1/1	0.99	0.05	35,35,35,35	0
4	CU	AAA	602	1/1	1.00	0.01	23,23,23,23	0
4	CU	AAA	603	1/1	1.00	0.01	23,23,23,23	0
4	CU	AAA	604	1/1	1.00	0.02	27,27,27,27	0
4	CU	BBB	601	1/1	1.00	0.01	25,25,25,25	0
4	CU	BBB	602	1/1	1.00	0.01	27,27,27,27	0
4	CU	BBB	603	1/1	1.00	0.01	26,26,26,26	0
4	CU	BBB	604	1/1	1.00	0.04	31,31,31,31	0
4	CU	AAA	601	1/1	1.00	0.02	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

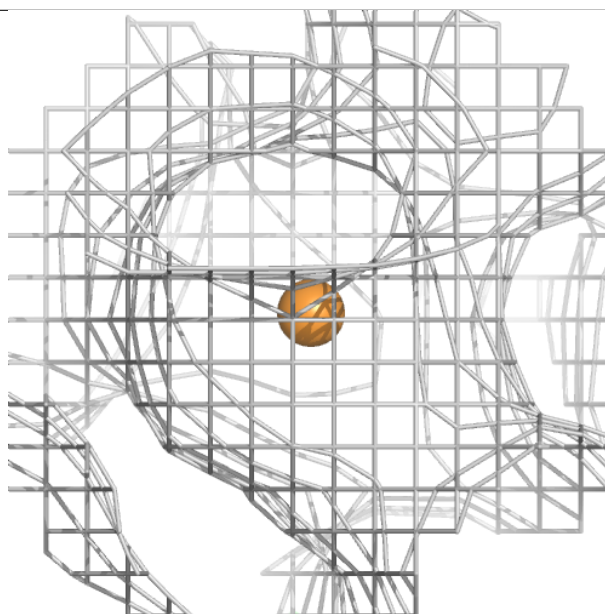
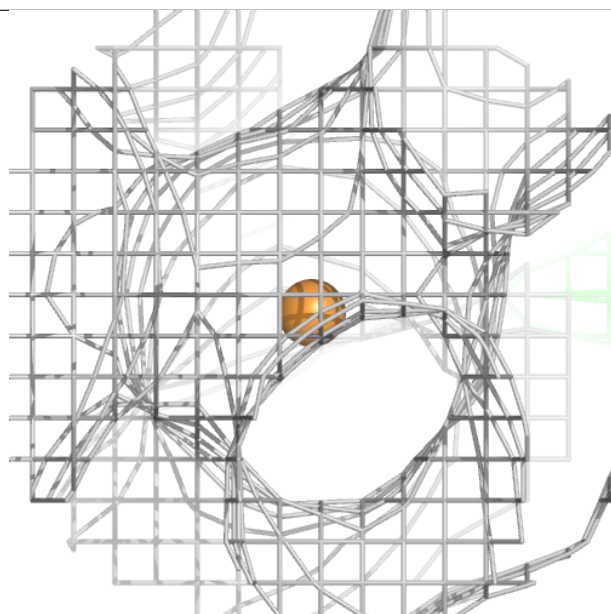
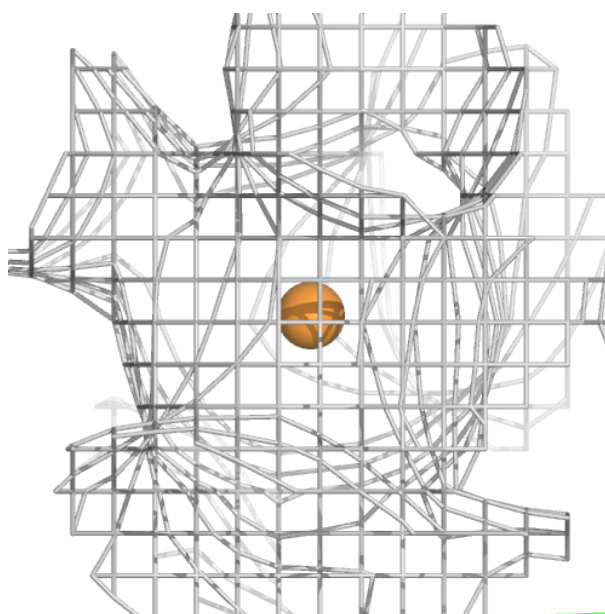
Electron density around CU AAA 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



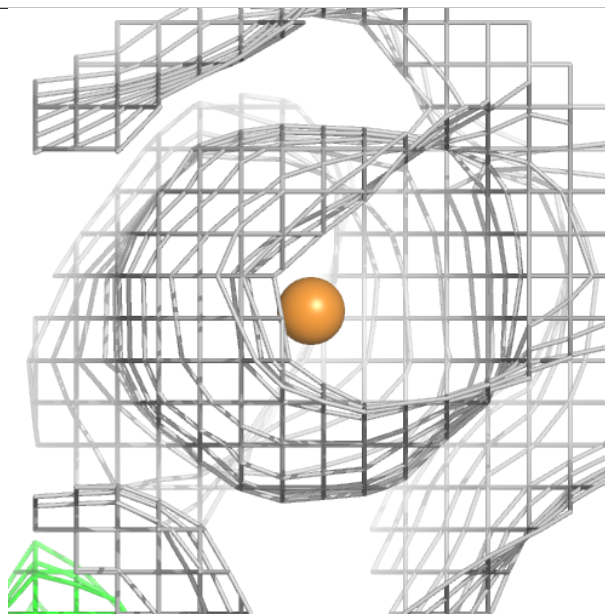
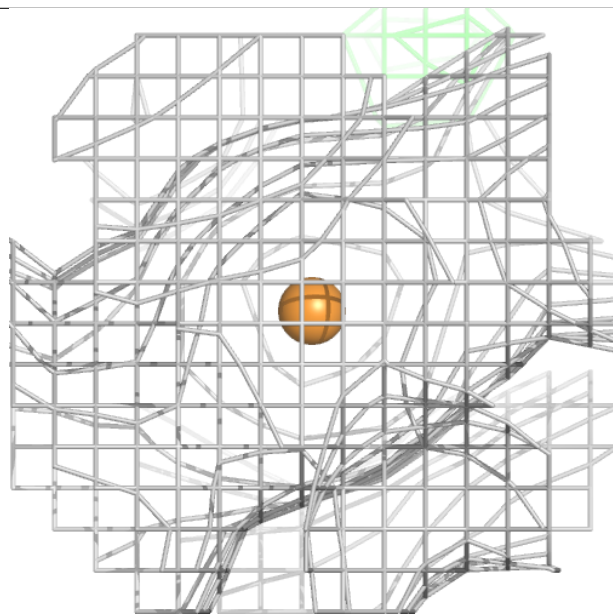
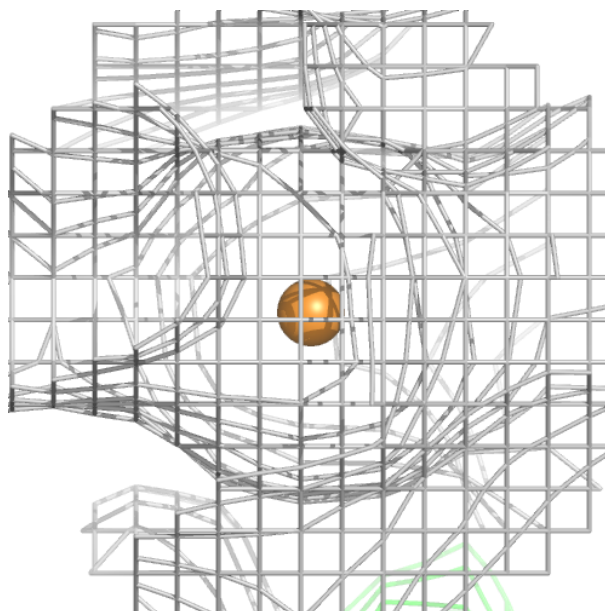
Electron density around CU AAA 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



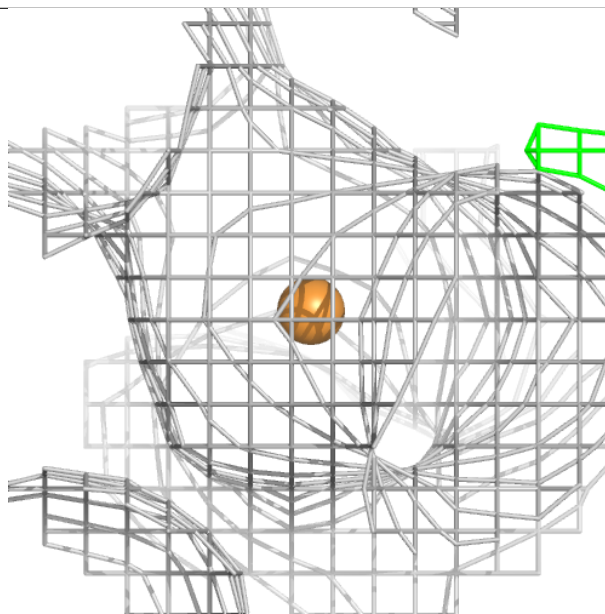
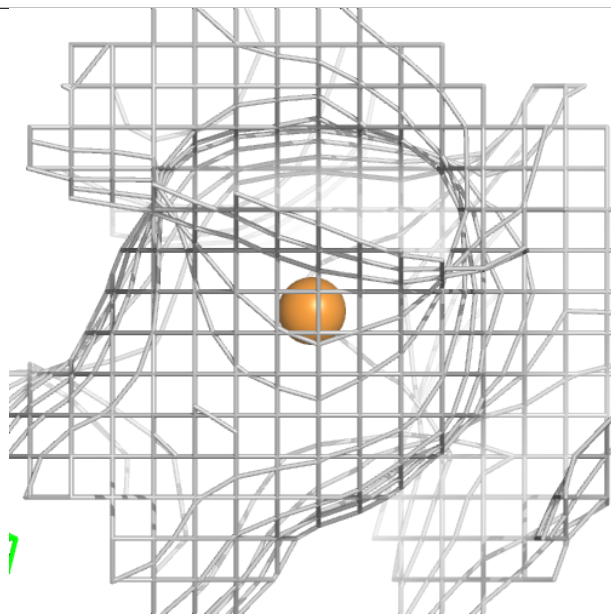
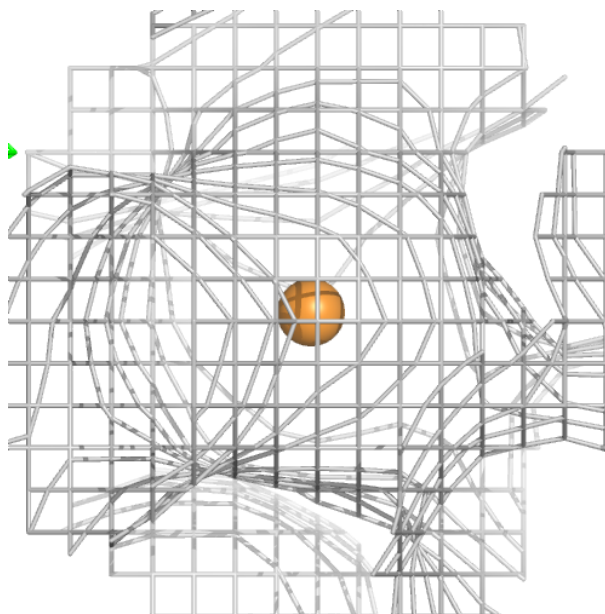
Electron density around CU AAA 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



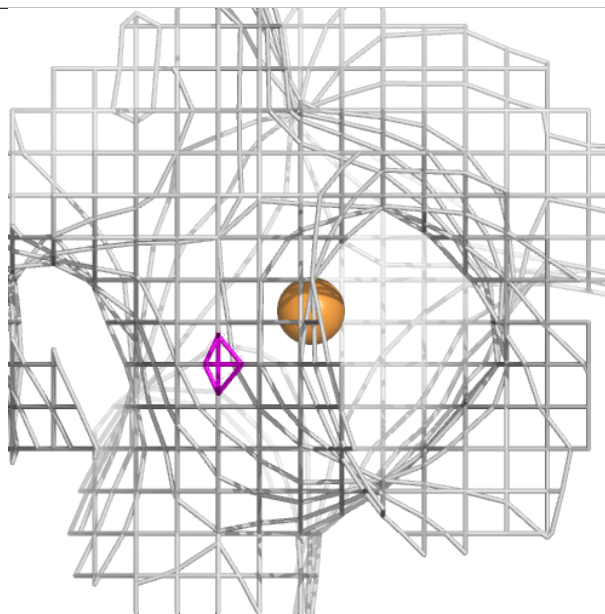
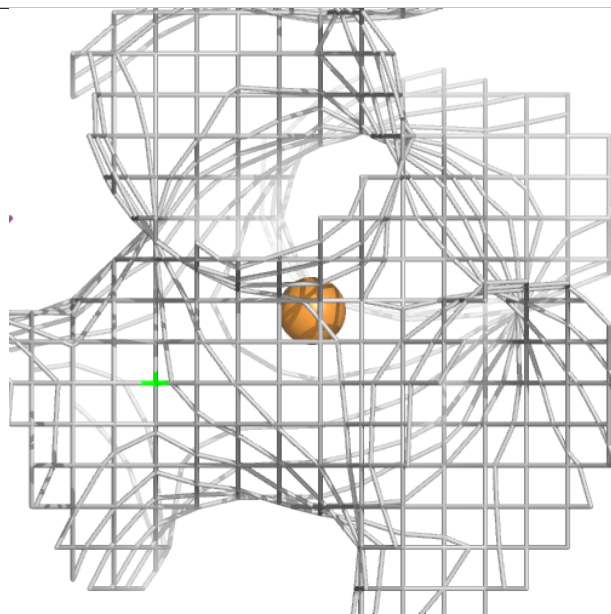
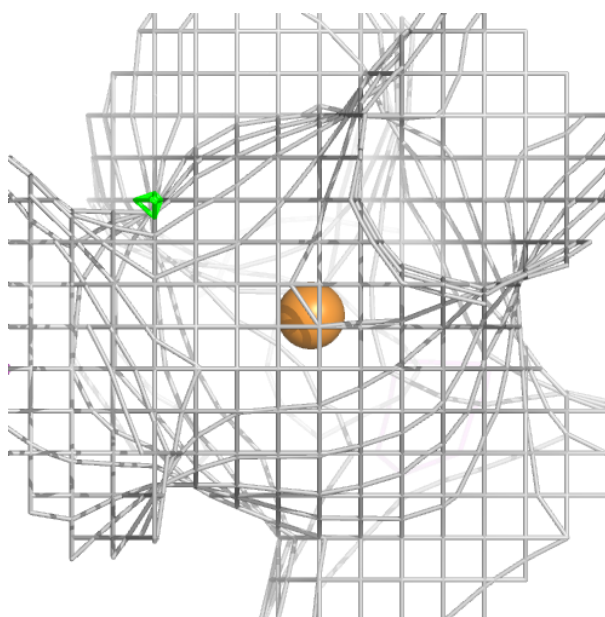
Electron density around CU BBB 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



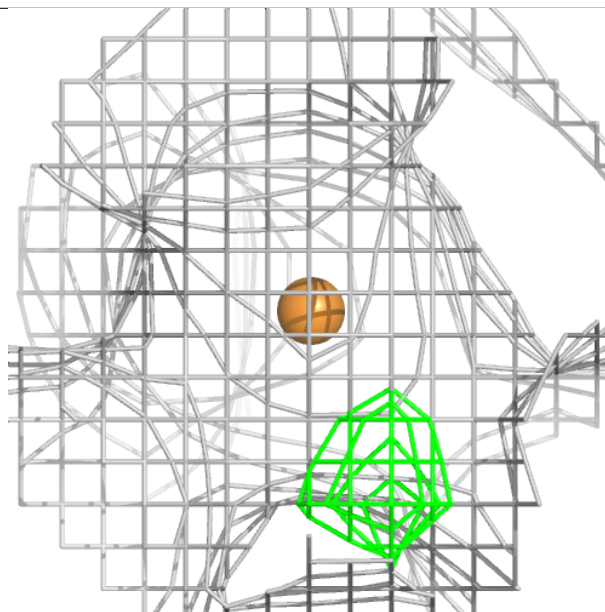
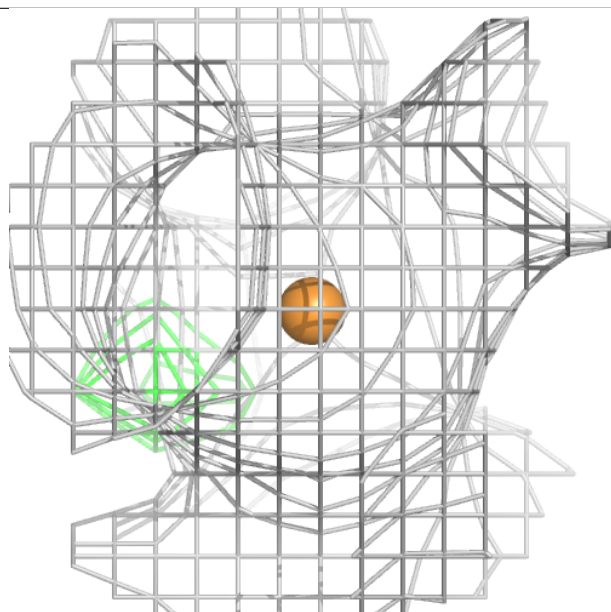
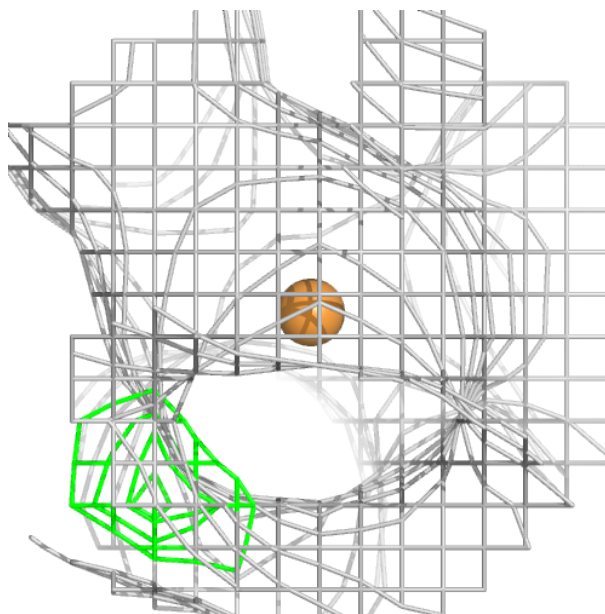
Electron density around CU BBB 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



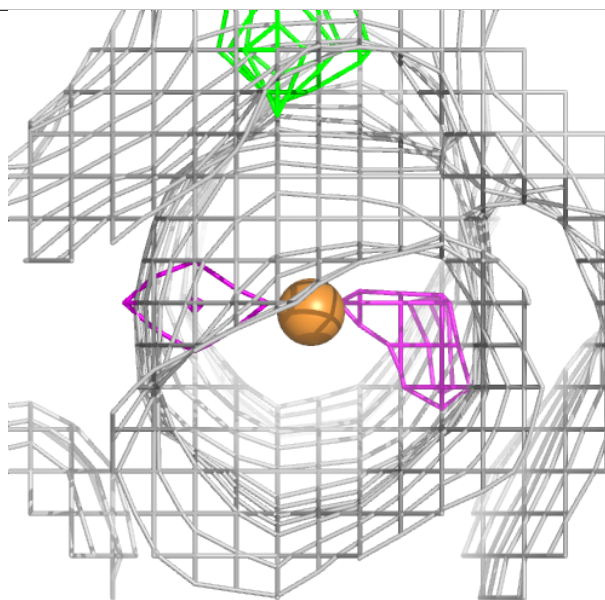
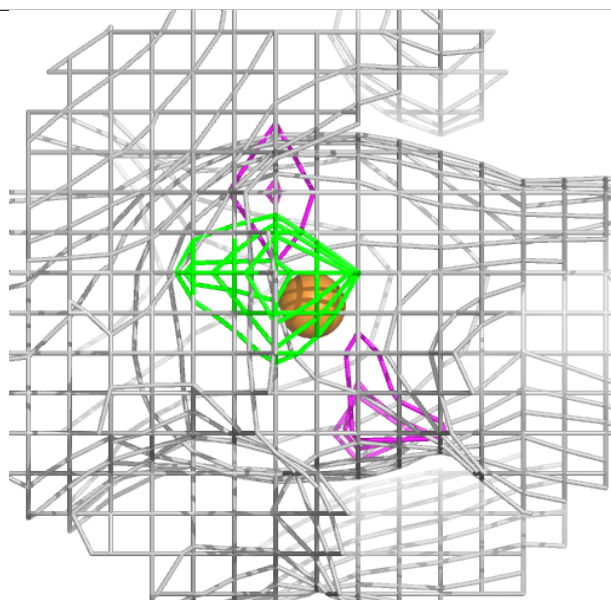
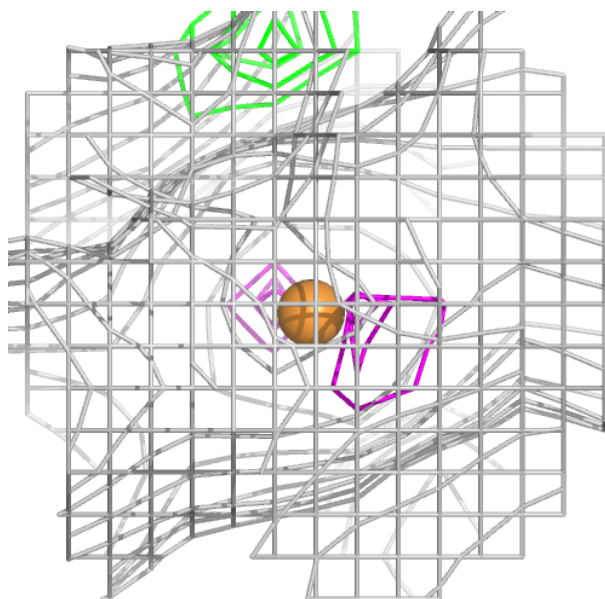
Electron density around CU BBB 603:

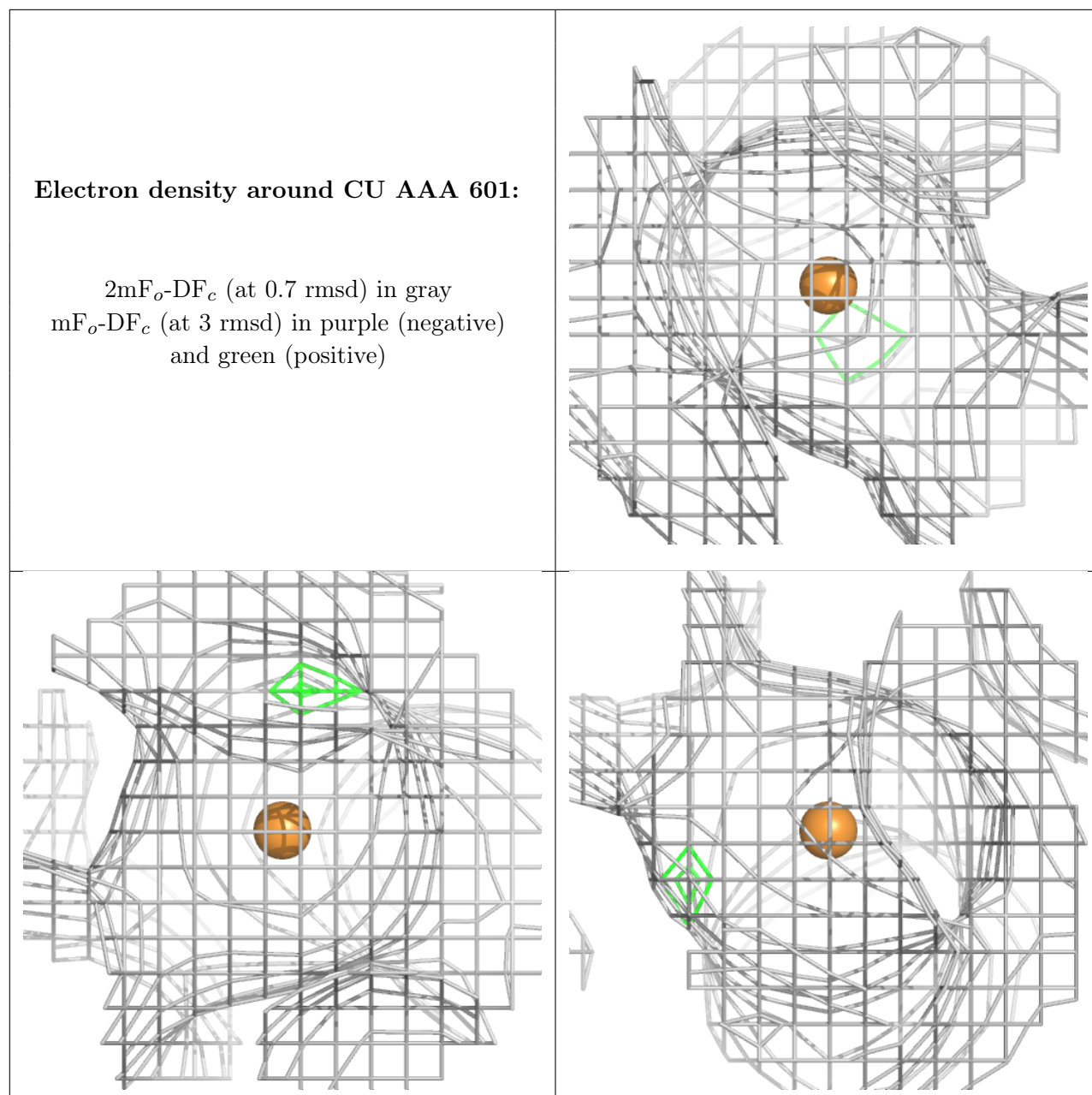
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU BBB 604:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.